

Acetic acid, nitro-, methyl ester

Other names:	Methyl nitroacetate Nitroacetic acid methyl ester Methyl 2-nitroacetate Methyl a-nitroacetate
Inchi:	InChI=1S/C3H5NO4/c1-8-3(5)2-4(6)7/h2H2,1H3
InchiKey:	ALBSWLMUHHZLLR-UHFFFAOYSA-N
Formula:	C3H5NO4
SMILES:	COC(=O)C[N+](=O)[O-]
Mol. weight [g/mol]:	119.08
CAS:	2483-57-0

Physical Properties

Property code	Value	Unit	Source
chl	-1431.10 ± 0.30	kJ/mol	NIST Webbook
chl	-1432.80 ± 0.30	kJ/mol	NIST Webbook
gf	-223.99	kJ/mol	Joback Method
hf	-360.81	kJ/mol	Joback Method
hfus	17.67	kJ/mol	Joback Method
hvap	48.02	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	-0.564		Crippen Method
mcvol	77.990	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	496.17	K	Joback Method
tc	715.35	K	Joback Method
tf	339.34	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.79	J/mol×K	496.17	Joback Method
cpg	168.76	J/mol×K	532.70	Joback Method
cpg	175.41	J/mol×K	569.23	Joback Method

cpg	181.74	J/mol×K	605.76	Joback Method
cpg	187.74	J/mol×K	642.29	Joback Method
cpg	193.40	J/mol×K	678.82	Joback Method
cpg	198.72	J/mol×K	715.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	3.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2483570&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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